21st NIST Computer Modeling Workshop
co-sponsored by ASTM Committees C01 and C09

DATE and LOCATION

Wednesday August 11, 2010 to Friday August 13, 2010
Lecture Room E, Building 101
National Institute of Standards and Technology
Gaithersburg, Maryland 20899 USA

INSTRUCTORS

Jeff Bullard (coordinator), Dale Bentz, Edward Garboczi, Nicos Martys, Paul Stutzman,
NIST Materials and Construction Research Division
Valerie Coffman, Jonathan Guyer, NIST Materials Science and Engineering Laboratory
Jeff Thomas, Northwestern University, Civil Engineering
Hegoi Manzano, Kitty Jia, Mostafa Youssef, Rouzbeh Shahsavari, Massachusetts
Institute of Technology, Civil and Environmental Engineering

GENERAL DESCRIPTION

The workshop lectures will cover computational and experimental materials science of concrete topics, including simulation of microstructural development and prediction of physical properties. "Microstructure" ranges from nanometer to meter length scales, while physical properties include pressure-driven fluid flow, rheology, mechanical properties, neutron scattering, scanning electron microscopy, and various X-radiation probes like diffraction and tomography. Close cooperation between computation and experiment is crucial for making progress in the materials science of concrete and so is an emphasis of the workshop. The workshop will have a mix of tutorial lectures and short 15-minute talks by the participants describing their technical work.

WORKSHOP SCHEDULE

<u>WEDNESDAY August 11, 2010   Lecture Room E, Administration Building</u>

8:30-8:45 Welcome and Orientation   Jeff Bullard
8:45-9:30 Lecture No. 1   Ed Garboczi
Principles of modeling cement and concrete

9:30-9:40 Break

9:40-10:40 Lecture No. 2   Paul Stutzman
Microstructure in Portland Cement Paste and Concrete

10:40-11:00 Break

11:00-12:00 Lecture No. 3   Jeff Bullard
Hydration Modeling: HydratiCA

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:15 Lecture No. 4   Jeff Bullard
Thermodynamic Modeling of Hydration and Microstructure Development

2:15-2:45 Break

2:45-3:45 Lecture No. 5   Nicos Martys
Computational Rheology and Transport Modeling

3:45-4:00 Break
4:00-5:00 Workshop Participants Presentations (4)
5:00 Bus leaves for Holiday Inn

<u>THURSDAY August 12, 2010   Lecture Room E, Administration Building</u>

8:30-9:30 Lecture No. 6   Jeff Thomas
Neutron Scattering and Hydration Modeling of Cementitious Materials

9:30-9:45 Break

9:45-10:45 Lecture No. 7   Valerie Coffman
Object-Oriented Finite Elements (OOF) for Modeling Materials Behavior

10:45-11:00 Break

11:00-12:00 Lecture No. 8   Dale Bentz
Early Age Cracking of Concrete: Causes and Mitigation

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:15 Lecture No. 9   Jonathan Guyer
Phase Field Modeling: Applications to Corrosion

2:15-2:45 Lecture No. 10   Jonathan Guyer
FiPy: A Software Package for Solving PDEs

2:45-3:00 Break

3:00-4:00 Workshop Participant Presentations (4)

4:00 Bus (or walk) to NIST Center for Neutron Research (NCNR)
4:05-5:00 Tour of NCNR
5:00 Bus back to Holiday Inn (from NCNR)

FRIDAY August 13, 2010   Lecture Room E, Administration Building

8:30-9:15 Lecture No. 11   Hegoi Manzano
Ab Initio Techniques for Investigating Structure of Cement Minerals

9:15-9:45 Lecture No. 12   Kitty Jia
Monte Carlo Modeling of Confined Water Thermodynamics

9:45-10:00 Break

10:00-10:30 Lecture No. 13   Mostafa Youssef
Molecular Dynamics Simulations for Water in C-S-H

10:30-11:00 Lecture No. 14   R. Shahsavari
C-S-H Texture from Nanometers to Micrometers

11:00-11:15 Break

11:15-12:00 Workshop Participant Presentations (3)

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:30 Workshop Participant Presentations (5)

2:30 Walk to Center for Nanoscale Science and Technology (CNST)
2:40-3:40 Tour of CNST

4:00-5:00 Workshop Participant Presentations (4)
5:00 Bus leaves for Holiday Inn
5:00 and 5:30 NIST Shuttle leaves for Shady Grove Metro to downtown Washington, DC

Registration

The list of workshop participants will be finalized by **July 20, 2010**, which is the application deadline. On-line registration is available and is the preferred method of registration (http://concrete.nist.gov/monograph/, click button for "2010 Workshop," then "Registration"). If on-line registration is not used, then the enclosed form (see below) will need to be filled out for each potential participant and sent to the coordinator (post, fax, or e-mail) in lieu of using the on-line registration site. There is no registration fee.

Housing and Meals

A partial list of hotels near NIST is available on the workshop website. Many of these hotels offer shuttle services to and from NIST. Participants are also encouraged to use their favorite travel websites to search for special rates or other accommodations. Workshop participants are responsible for the costs of meals.

Getting to NIST

See the following web site for detailed information about getting to NIST (e.g., taxis, shuttles, restaurants) –http://www.nist.gov/public_affairs/visitor/visitor.htm. If workshop participants land in Dulles International Airport, a taxi can be taken directly to the Gaithersburg Holiday Inn at a cost of about $70.00. Those persons flying into Reagan National Airport can take the Metro underground train directly to the Shady Grove stop in Gaithersburg (about $3-$6, depending on time of day—see signs in Airport station--Yellow line to Gallery Place, Red line to Shady Grove). A taxi may be taken from there to the Gaithersburg for about $15.00.

Alternatively, a taxi can be taken directly to the hotel from Reagan National for about $65.00. From Baltimore Washington International Airport, taxis cost about $90.00 to Gaithersburg. Shuttles are somewhat cheaper – see the airport web site for details. Driving directions to NIST are included on the NIST web site.

Security

All workshop attendees must have a picture I.D. with them to be able to enter the gates, either riding on the bus from Holiday Inn or by themselves. A U.S. driver's license or passport is fine. A temporary NIST badge will be given to you on your first entrance to NIST, which, along with your picture I.D., will allow entrance into NIST for the rest of the workshop. So don't throw it away! And please wear the NIST badge at all times while within NIST.

Note: Non-US citizens are required to give some additional information. You will see a place for this on the on-line registration, and on the form below.

Direct all questions to the Workshop coordinator:
Jeffrey W. Bullard
NIST, 100 Bureau Drive, Stop 8615, Gaithersburg, MD 20899-8615 USA
Phone: (301) 975-5725 (office), (301) 990-6891 (fax)
Electronic Mail: jeffrey.bullard@nist.gov

Please register on-line (preferable) at http://concrete.nist.gov/monograph/, or else return this form to the workshop coordinator, no later than July 20, 2010.

21st NIST Computer Modeling Workshop Registration Form

Full Name and Title:

Institutional Affiliation:

Citizenship (necessary for NIST security):

Research Advisor (if student or post-doc):

Mailing Address:

Phone Number:

Fax Number:

E-Mail (<u>please print clearly</u>):

Title for your 15-minute presentation on your technical work:

Purpose for coming to the Computer Modeling Workshop:

If you are not a US citizen, please supply the following additional information:

Date of birth (month-day-year):

City and country of birth:

Passport number and issuing country:

Employer/sponsor:

Citizenship (include dual citizenship if applicable):

Country of residence:

Are you a US permanent resident?

Gender: